AMENDMENTS TO THE CLAIMS

1. (CURRENTLY AMENDED) A computer-implemented method of predicting functional similarity between two molecules comprising:

deriving a first one-dimensional representation of a first molecule with a known chemical behavior from distances between selected atoms of said first molecule, said one dimensional representation comprising a string of atoms, each atom of said string having a selected type, a selected width, and a selected position along said string ~~wherein the selected atoms of the first molecule are assigned positions in the first one-dimensional representation~~;

deriving a second one-dimensional representation of a second molecule with an unknown chemical behavior from distances between selected atoms of said second molecule, said one dimensional representation comprising a string of atoms, each atom of said string having a selected type, a selected width, and a selected position along said string ~~wherein the selected atoms of the second molecule are assigned positions in the second one-dimensional representation~~; and

comparing said one dimensional representations, wherein the comparing comprises:

aligning the one dimensional representations such that the position of an atom of a first selected type in the first one dimensional representation coincides with the position of an atom of the first selected type in the second one-dimensional representation; and

evaluating the amount of overlap between atoms of each selected type in the first one-dimensional representation and atoms of the same type in the second one-dimensional representation; and

identifying the second molecule as likely to have similar chemical behavior as the first molecule based on said comparing.

2-3. (CANCELED)

4. (CURRENTLY AMENDED) The method of Claim ~~3~~1, wherein said ~~linear~~ positions in the first one-dimensional representation are selected to reduce the deviation between

relative positions of ~~said plurality of selected~~the atoms in the string of atoms ~~along a line~~ and three dimensional distances between ~~said plurality of~~the atoms in said first molecule.

5-6. (CANCELED)

7. (CURRENTLY AMENDED) The method of Claim ~~6~~1, wherein the atoms of the first selected type in the first and second one-dimensional representations ~~said matched atoms~~ have the same element type.

8. (CURRENTLY AMENDED) The method of Claim 7, wherein the atoms of the first selected type in the first and second one-dimensional representations ~~said matched atoms~~ have the same hybridization state.

9. (ORIGINAL) The method of Claim 1, wherein at least some of said distances are derived from molecular topology.

10. (ORIGINAL) The method of Claim 9, wherein at least some of said distances are derived from bond counts.

11. (ORIGINAL) The method of Claim 1, wherein at least some of said distances are derived from three dimensional atomic coordinates.

12-17. (CANCELED)

18. (CURRENTLY AMENDED) ~~A computer-implemented method of representing a non-linear three dimensional configuration of a molecule made up of a plurality of bonded atoms, said method comprising assigning, to at least some of said atoms, a position along a line so as to define a set of linear distances between each of said selected atoms~~The method of claim 1, wherein at least some ~~of said linear distances~~relative positions of the atoms in the one-dimensional representations are not equal to ~~the~~ corresponding three dimensional distances between the same atoms in ~~said~~ the molecules.

19-21. (CANCELED)

22. (CURRENTLY AMENDED) A computer-implemented method of selecting for further testing and analysis a subset of molecules from a library of molecular structures, said method comprising:

storing ~~linear~~ one-dimensional representations of said molecular structures in a database, said ~~linear~~ one-dimensional representations being derived from three

dimensional distances or topological distances between atoms of said molecular structures, ~~wherein at least some of the atoms of each molecular structure are assigned positions in the respective linear representations~~wherein said one dimensional representations comprise strings of atoms, each atom of each string having a selected type, a selected width, and a selected position along the string;

deriving a ~~linear~~ one-dimensional representation of a molecule having known biochemical activity from three dimensional distances or topological distances between atoms of said molecule; wherein at least some of the atoms of said molecule are assigned positions in ~~the respective linear~~a one-dimensional representations of the molecule, wherein the one dimensional representation of the molecule comprises a string of atoms, each atom of the string having a selected type, a selected width, and a selected position along the string;

comparing said ~~linear~~ one-dimensional representation of said molecule having known biochemical activity with said ~~linear~~ one-dimensional representations of said molecular structures in said database, wherein the comparing comprises:

aligning the one dimensional representation of said molecule with the one-dimensional representations of said molecular structures such that the position of an atom of a first selected type in the one dimensional representation of said molecule coincides with the position of an atom of the first selected type in the one-dimensional representations of said molecular structures; and

evaluating the amount of overlap between atoms of each selected type in the one-dimensional representation of said molecule and atoms of the same type in the one-dimensional representation of said molecular structures; and

identifying a molecular structure of said molecular structures as likely to have similar chemical behavior as said molecule based on said comparing.

23-29. (CANCELED)

30. (CURRENTLY AMENDED) A computer readable storage medium having stored thereon structural representations of molecules for retrieval by a computer implemented molecular screening program, wherein at least one of said structural representations comprises a

list of selected atoms in said molecule, wherein each of said selected atoms is associated with an atom type ~~and a scalar value~~, a selected width, and a selected position along a one-dimensional string of atoms.

31. (CURRENTLY AMENDED) The ~~method~~ storage medium of Claim 30, wherein said selected position ~~scalar value~~ is derived from distances between said selected atoms in said molecule.

32. (CURRENTLY AMENDED) The ~~method~~ storage medium of Claim 31, wherein said distances comprise three dimensional distances.

33. (CURRENTLY AMENDED) The ~~method~~ storage medium of Claim 31, wherein said distances comprise topological distances.

34-35. (CANCELED)

SUMMARY OF INTERVIEW

The Applicants wish to thank the Examiner for a series of telephonic interviews conducted from March to June 2006. The Examiner provided helpful suggestions for clarifying the language in Claim 1 in order to place the claim in condition for allowance. The presently amended claims are the culmination of all of the Examiner's comments and are believed to address all of the concerns and suggestions raised.